Simulating Quantum Computing on Traditional HPC Systems: Developing Tomorrow's Quantum Algorithms on Today's CMOS Hardware

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25 Years of High Performance Computing, Storage, Networking Solutions

1990

1998
Telstra Digital Video Network
Supplied Video Server equipment

2000

2000
Animal Logic
Render Farm delivered for the "Matrix" movie trilogy

2004
TataSky DTH India
Supplied Video Logging solution

2005
Thales Defence
Supplied Image Generators for the ASLAV simulators

2007
Victorian Partnership for Advance Computing
Supplied HPC Cluster for Advance Computing

2010

2009
CSIRO
(10th in Green500 ranking)
Supplied Australia's first GPU Cluster ("Bragg")

2011
Australian Stock Exchange (ASX)
Supplied Infiniband equipment

2011
Fox Broadcasting USA
Supplied Video Logging solution

2012
Fujitsu
Supplied Infiniband Network for Australia's largest Supercomputer ("Raijin")

2013
Digital Cinema Systems
Upgraded 150 Independent Cinemas in ANZ region

2014
University of Queensland
FlashLite HPC cluster system for high data throughput

2015
Thales Defence
Delivered High Fidelity Solution for Australian Army Tiger Helicopter Simulator

2015
Futuris
XENON drive high performance innovation

2016
Garvan Institute of Medical Research
NVMe solution that enables high data throughput

2016
Oil Search
Deployed Intel® CAS to speed reservoir modeling

2017
The Walter and Eliza Hall Institute
Private Cloud For Next Generation Cancer, Disease & Medical Research

2017
NCI
Supercomputer dedicated to scientific research & technology innovation

2018
Harrison.ai
Democratising reproductive healthcare through AI

2019
Pawsey Supercomputing Centre
New GPU Cluster for Pawsey Supercomputing Centre, Perth WA

2020

2020
CSL Limited
Professional Services HPC Cluster

2020
Todd Energy
HPC Cluster for Todd Energy in Wellington, NZ

2021
XENON Cluster Stack
XENON launches containerised HPC solution

2021
Murdoch Children's Research Institute
Implementation of a backup solution

2021
Hong Kong Uni HPC
Deployed HPC Cluster with XENON Cluster Stack for HKU

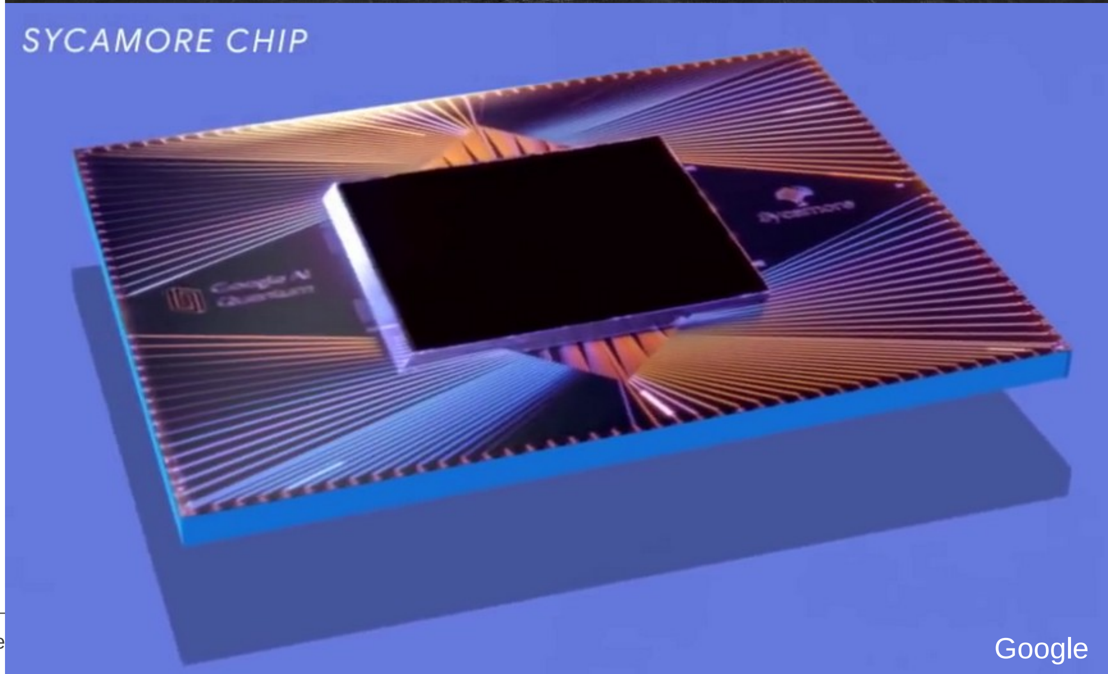
Our customised technology solutions and products are designed to tackle the most data intensive and complex visualisation challenges, allowing our clients to do great new things, and break new ground in their respective fields.

25 YRS OF HPC XENON® High Performance Computing

Why Quantum Computing?

- **Cryptography:**
  Factorisation of large numbers (to break encryption algorithms)
- **Optimisation:**
  Optimisation problems in science, finance, logistics
  NP-hard, NP-complete problems, e.g. Travelling Salesman problem
- **Quantum Communication and Networking**
  Secure communication
  Nobel Prize Physics 2022
- **Quantum Machine Learning/AI**
- **Quantum Physics and Chemistry:**
  Simulating quantum systems with “Variational Quantum Eigensolvers”

IBM



Google

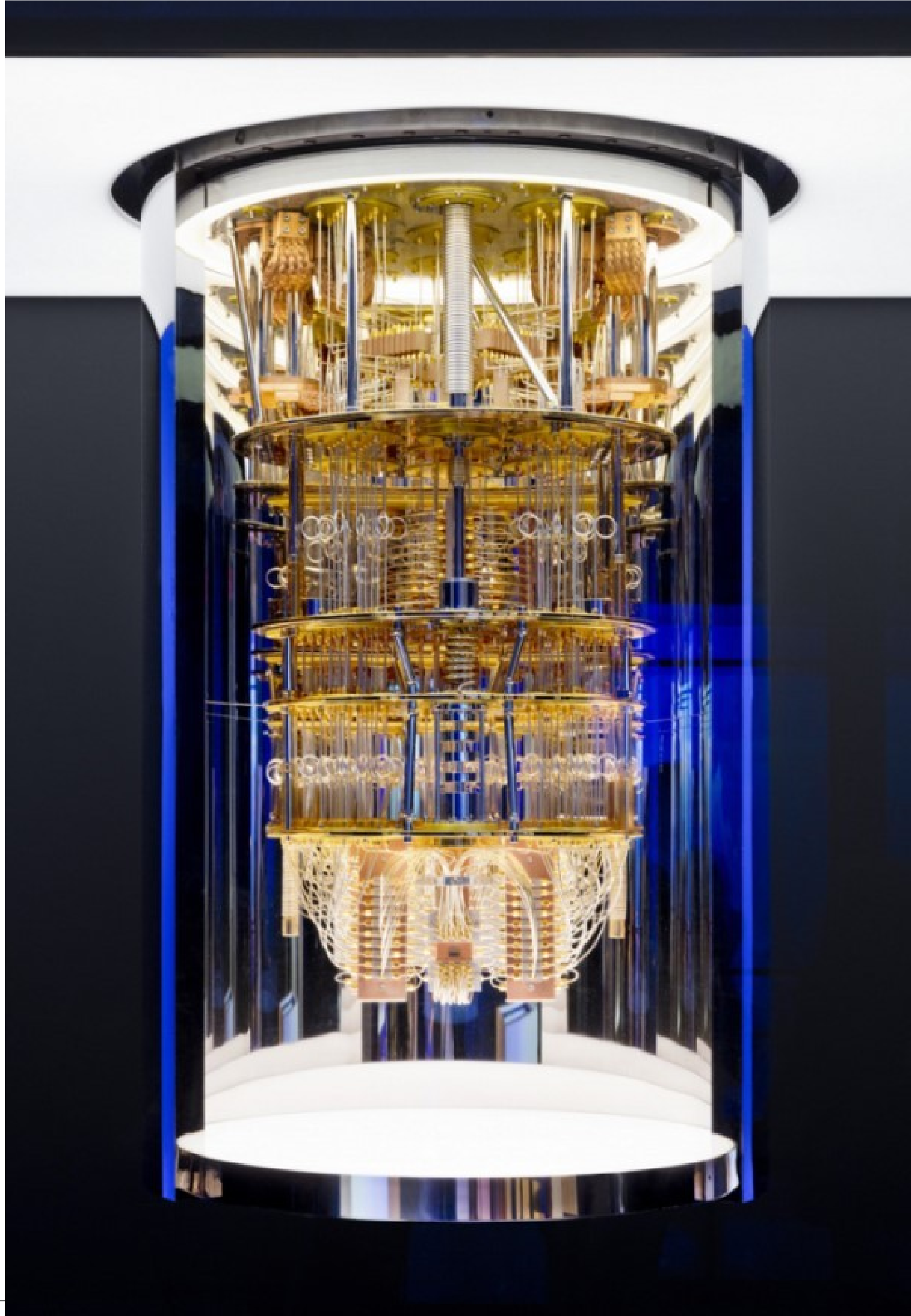
Quantum Computing Hardware Basics

Qubits

- cooper pairs in Josephson junctions/SQUIDs
- ions in electromagnetic traps manipulated with laser pulses,
- nuclear spins of molecules manipulated with nuclear magnetic resonance
- single photons in non-linear optical media
- ...

Challenges

- Noise suppression
  - Cooling: liquid He
  - Isolation: Shielding electric and magnetic fields
- Minimise crosstalk between qubits
- Methods to manipulate, measure and entangle qubits
- Increase coherence time: The duration for which the quantum state keeps its quantum nature (i.e. the time available for computing)
- Increase “Quantum Volume”: metric including capabilities and error rates

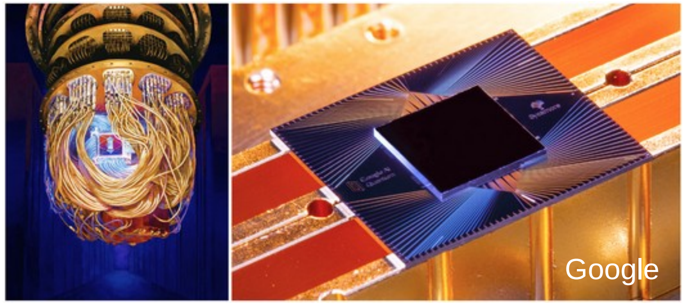


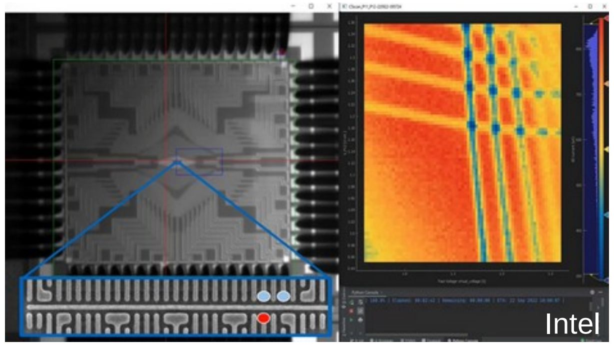
IBM

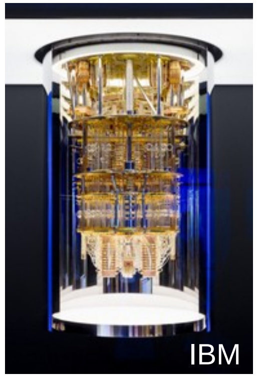
Available Systems

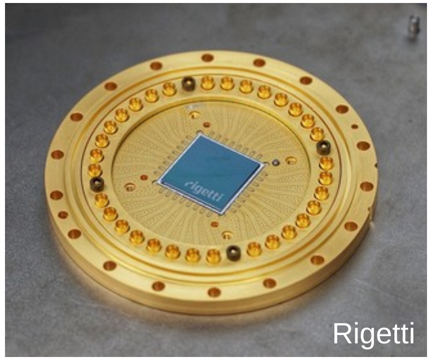
Noisy intermediate-scale quantum (NISQ) technology

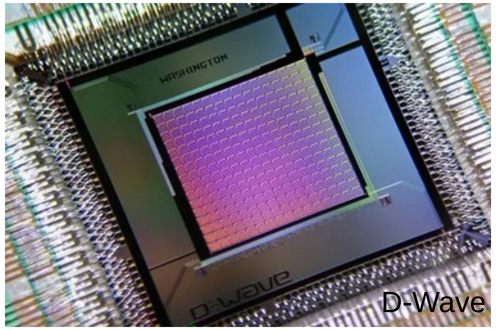
- Quantum Brilliance: nitrogen-vacancy (NV) centres in diamonds
- Silicon Quantum Computing: quantum integrated circuit on silicon
- Alpine Quantum Technologies: Trapped Ions
- IBM Q: various systems based on SQUIDs and transmons
- Google: Superconducting Transmon
- IonQ: Trapped Ytterbium Ions
- Intel: several approaches including superconducting qubits and spin qubits
- Pasqal: ordered neutral atoms in 2D and 3D arrays
- Quantinuum: Trapped Ions
- Quandela: Photonics
- Rigetti: various systems based on superconducting qubits and transmons
- SpinQ: Nuclear Magnetic Resonance
- D-Wave: Quantum Annealing
- various universities and new startups











Quantum Computing 101

Classical Computing:

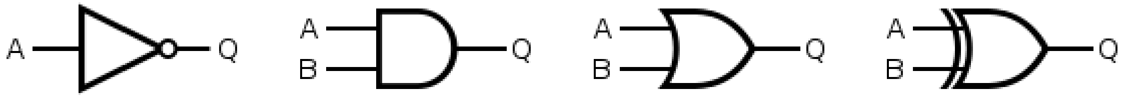
- A bit is either 0 or 1
  (in some form of physical representation: charge accumulation in CMOS transistors, electrons/charge in flash chips/SSDs, magnetization in HDDs and MRAM, crystalline/amorphous phase in 3D-Xpoint/Optane, resistance in RRAM,...)
- We can set it to either 0 or 1
- We can read (measure) if it is 0 or 1
- Bits don't interact (unless they do, which causes noise and errors)
- Mathematical representation:
  - Each bit is 0 or 1
  - Operators: take one or multiple bits as input and generate one or multiple bits as output (can be represented as matrices)

Quantum computing:

- A qubit is 0 or 1 or both (a mixture) at the same time (superposition)
- We can set it to either 0 or 1 or a mixture of both
- We can read (measure) if it is 0 or 1 and we will get either 0 or 1 with a certain probability
- Qubits can be correlated "entangled" causing nonlocality
  (Einstein called it "spukhafte Fernwirkung" - "spooky action at a distance" and argued with Schrödinger – and himself – about it.)
- Mathematical representation:
  - Two orthonormal basis states: $|0\rangle$ and $|1\rangle$
  - Two-state quantum system: expressed as a linear superposition $\psi = \alpha^*|0\rangle + \beta^*|1\rangle$ with $|\alpha|^2+|\beta|^2=1$
  - Classical representation: two-element complex-value array as $[\alpha\ \beta]^T$
  - Operators: matrices

Quantum Computing 102

Logic Gates in Classical Computing:



NOT

Input	Output
A	Q
0	1
1	0

AND

Input		Output
A	B	Q
0	0	0
0	1	0
1	0	0
1	1	1

OR

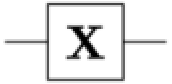
Input		Output
A	B	Q
0	0	0
0	1	1
1	0	1
1	1	1

XOR

Input		Output
A	B	Q
0	0	1
0	1	0
1	0	0
1	1	1

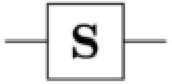
Logic Gates in Quantum computing:

Pauli-X



$$X|0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

Phase



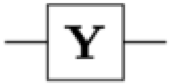
$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad Z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

Hadamard

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} = |+\rangle$$

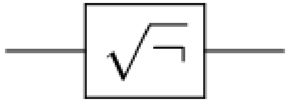
Other gates:

Pauli-Y



Pauli-Z

Square root



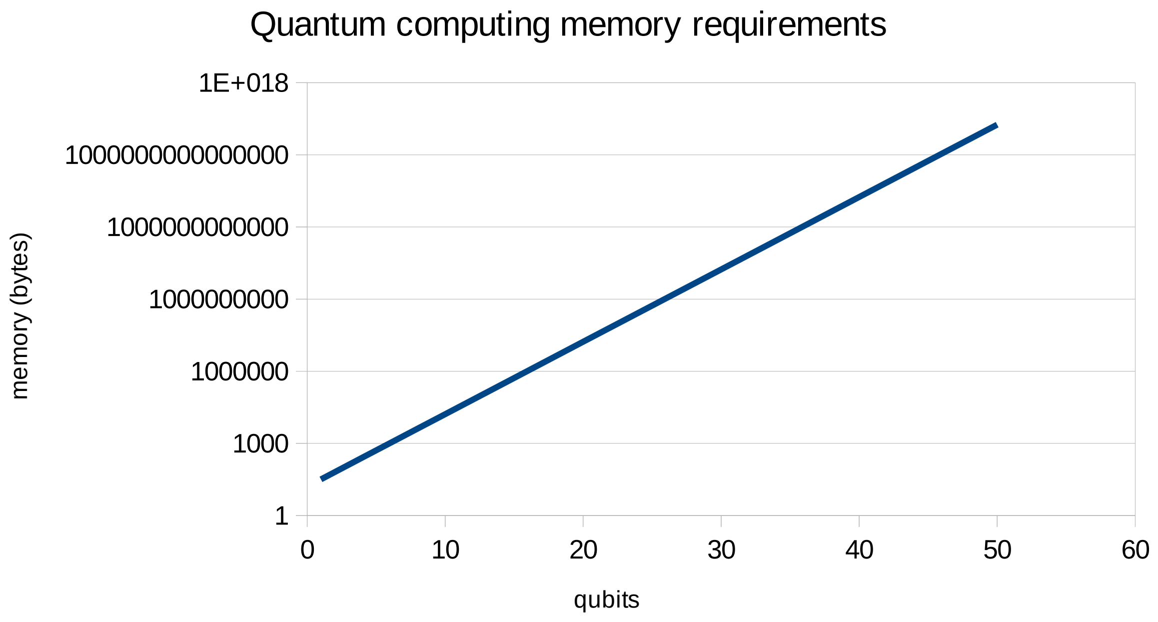
Simulating Quantum Computers

Typical assumptions

- Simulate perfect qubits
- Defect free
- Noise free
- Infinite coherence times
- Error free
- Perfect fidelity

Requirements

- Memory requirements for N qubits = $2^N * 2 * 8$ bytes (double precision)
  - 31 qubits: 34.4 GB
  - 40 qubits: 17.5 TB
  - 50 qubits: 18.01 PB
  - 100 qubits: $2.03*10^{16}$ PB
- CPU requirements for state change of N qubits = 2^N operations
- Runtime scales linearly with quantum circuit depth
- Use HPC systems – with lots of memory and accelerators!



Quantum Simulation Services and Toolkits

- **IBM Qiskit**
  Complete open source software stack including
  - tools for creating quantum programs and running them on superconducting qubits and trapped ion systems.
  - simulators including realistic noise
  - frameworks for optimisation, finance, machine learning, quantum chemistry
- **Google Cirq**
  Programs can run in local simulators or against hardware supplied by IonQ, Pasqal,[6] Rigetti, and AQT.
  Various projects leveraging Cirq including “TensorFlow Quantum” for hybrid classical-quantum machine learning algorithms.
- **NVIDIA cuQuantum:** multi-GPU multi-node solution for quantum circuit simulation, integrates with Cirq, Qiskit
- **Q-CTRL:** Quantum infrastructure software
- **Amazon Braket:**
  Quantum algorithm development environment and simulator, access to quantum computers built by IonQ, Rigetti, Xanadu, QuEra, Oxford Quantum Circuits, D-Wave
- **Intel Quantum Simulator:** Open source simulator of quantum circuits optimized for multi-core and multi-nodes architectures.
- **Atos QLM:** Programming development platform and quantum simulator.
- **Pasqal:** Emulation of up to 100 qubits in 2D and 3D arrays PASQAL’s quantum processors on 10x NVIDIA DGX Systems
- High Level Quantum Programming Languages
  - Silq
  - Classiq

Quantum Algorithms

- https://quantumalgorithmzoo.org/

Next Steps

Improve Quantum Computers

- Increase number of qubits and scalability
- Reduce noise and error rates, improve error correction
- Increase coherence time
- Reduce complexity and cost
- Race to Quantum Supremacy (“Are we there yet?”)

Improve Simulators

- Simulate ideal quantum computers
- Simulate realistic quantum computers including characteristics of the specific qubit implementation and noise
- Accelerate quantum simulators (e.g. with GPUs)

We need new algorithms!

- Use quantum:
  - Pure quantum algorithms
  - Hybrid classical-quantum algorithms
  - Quantum AI (!?)
- Beat quantum:
  - Post-quantum Cryptography (NIST competition)

We need more

- Expertise
- Investment
- Strategy
- Commercialisation

How to get out of NISQ?

- **Factorisation:**
  To factor a composite number of 2048 bits would require around 10,000 qubits, 2.23 trillion quantum gates, and “a quantum circuit depth of 1.8 trillion”, Fujitsu said in a statement. A sufficiently-large fault-tolerant quantum computer would need 104 days to crack RSA. [Fuji01]

Thank You

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